Course work: Exact diagonalization

Processing time: **Monday 17th of July 2023, 12PM – Friday 21st of July 2023, 11:59PM**

General information

This programming project serves as qualification for the final, oral exam of the lecture *Numerical Quantum Physics*. The problem has to be processed independently in the time frame denoted above and the solutions are to be uploaded into a `nextcloud` folder, shared with the registered students via mail. Please note that in order to accept the solution, the upload timestamp in the `nextcloud` folder is used. Any solution that is provided after the final submission deadline can not be considered and will be ignored. However, you do have the possibility to invalidate already submitted solutions until the submission deadline.

The solutions are to be provided via source code <u>and</u> a PDF document which contains a short documentation of the implemented functionality, as well as optional plots and interpretations depending on the particular problem. Reviewing the submitted solution, the source code will be executed using the standard libraries provided via the `init_modules.sh`-script provided on the lecture's home directory `/project/cip/2023-SS-NQP/init_modules.sh`, and the generated results are compared to the discussions and plots in the submitted documentation file. Any use of additional, external libraries rendering the submitted solution non-executable is thus not permitted.

The consultation of relevant literature is highly welcome but needs to be documented. You may also use example code provided in the lecture, available via the lecture's home directory `/project/cip/2023-SS-NQP/examples`. Indicate the use of external resources in the documentation file via proper citations, for instance using the LaTeX package `natbib` together with the `plainnat` bibliography style. In case you are using large language models, e.g., `ChatGPT`, the full dialog generating the respective contributions to your solution, concerning both code and documentation, needs to be stored and provided in a separate document. If large scale plagiarism without proper citation or documentation is detected, the solutions will be considered invalid.

Qualification for the final, oral exam requires to achieve at least 50 percent of the maximally possible points. The total grade will be obtained from equally weighting the marks of the coding project and the oral exam (and corrected by the bonus obtained from the exercises).

For questions please send an e-mail to the assigned supervisors:

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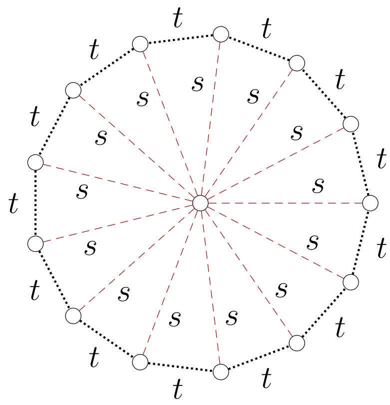

Figure 1: Wheel geometry with hopping amplitudes on the ring (t) and from the ring to the center (s).

Problem 1 Bose-Einstein condensation in wheels

Consider a lattice system of $L+1$ ($L \in \mathbb{N}$) hardcore bosonic degrees of freedom $\hat{h}_j^\dagger, \hat{h}_j$ satisfying the commutation relations

$$\left[\hat{h}_j, \hat{h}_l^\dagger\right] = \delta_{j,l}\left(1 - 2\hat{n}_j\right) \ , \quad \left[\hat{h}_j, \hat{h}_l\right] = \left[\hat{h}_j^\dagger, \hat{h}_l^\dagger\right] = 0 \ , \tag{1}$$

for all $j, l \in \{0, \dots L\}$ with $\hat{n}_j = \hat{h}_j^\dagger \hat{h}_j$ being the local hardcore bosonic occupation number operator. In the local occupation number basis $|n_j\rangle$, each lattice site can be either empty or occupied, i.e., $\hat{n}_j |n_j\rangle = n_j |n_j\rangle$ with $n_j \in \{0, 1\}$ (therefore the name hardcore bosons: there can not be more than one boson per lattice site!). The system we are considering describes a wheel geometry, i.e., there is one site j_c, let's choose the last site $j_c \equiv L$, which couples to all other lattice sites. Let us define $\hat{b}_j^{(\dagger)} = \hat{h}_j^{(\dagger)}$ for $j \neq j_c$ and $\hat{b}_{\odot,j}^{(\dagger)} = \hat{h}_{j_c}^{(\dagger)}$. Then, the Hamiltonian of the hardcore-bosonic wheel is given by

$$\hat{H}_\odot = -t \sum_{j=0}^{L-1} \left(\hat{b}_j^\dagger \hat{b}_{j+1} + \mathrm{h.c.}\right) - s \sum_{j=0}^{L-1} \left(\hat{b}_j^\dagger \hat{b}_\odot + \mathrm{h.c.}\right) \ , \tag{2}$$

with the ring hopping amplitude $t \geq 0$ and the ring-to-center hopping $s \geq 0$. The first sum implements periodic boundary conditions, i.e., the addition in the index labels: $j+1$ is to be understood modulo L. A sketch of the system is shown in fig. 1.

(a) **(4P)** Represent eq. (2) in matrix form

$$\hat{H}_\odot = \underline{\hat{\psi}}^\dagger \underline{\underline{H}}_\odot \underline{\hat{\psi}} \tag{3}$$

with operator-valued vectors $\underline{\hat{\psi}}^\dagger = \left(\hat{h}_0^\dagger, \hat{h}_1^\dagger, \cdots, \hat{h}_L^\dagger\right)$ and a $L+1 \times L+1$ matrix $\underline{\underline{H}}_\odot$. $\underline{\underline{H}}_\odot$ represents the single-particle Hamiltonian. Calculate the eigenvalues ε_n of $\underline{\underline{H}}_\odot$ as a function of the ratio of the coupling constants $s/t \in \geq 0$ for various system sizes L and plot your results in a so-called spaghetti plot, displaying the evolution of the eigenvalues $\varepsilon_n(s/t)$ as a function of $s/t \geq 0$.

(b) **(6P)** Write an exact diagonalization code, which represents eq. (2) in the occupation number basis $|n_0, n_1, \dots, n_L\rangle$ of the tensor-product Hilbert space of $L+1$ hardcore bosons, as well as the correlator $\hat{C}(j,l) = \hat{h}_j^\dagger \hat{h}_l$.

(c) **(6P)** Calculate the full spectrum (eigenstates are not required here) as a function of the ratio of the coupling constants $s/t \in \geq 0$ for various system sizes L, diagonalizing the matrix representation of eq. (2). Try to make L as large as possible (how could you further improve your code in principle) and plot the energies of the eigenstates $E_n(s/t)$ as a function of s/t in a spaghetti plot. Compare the evolution of the many-body spectrum to that of the single-particle case calculated in (a).

(d) **(4P)** Calculate the many-body ground states $|\psi_0\rangle$ of eq. (2) and evaluate the so-called single-particle reduced density matrix $\rho_{j,l}$

$$\rho_{j,l} = \langle\psi_0|\hat{C}(j,l)|\psi_0\rangle \ , \tag{4}$$

for all $j, l \in \{0, 1, \ldots, L\}$. Determine the largest eigenvalue n_0 of $\rho_{j,l}$, which is a measure for the number of hardcore bosons occupying the same single-particle state. Plot the condensate fraction n_0/N with the particle number $N = \sum_j \rho(j,j)$ as a function of s/t for various system sizes. Can you relate your results to the spectra plotted in (a) and (c)?